Gweicurculactone

123914-43-2 | DTXSID50154143

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%	Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.72	51.8	0.74	50.3	0.73	52.7	

Model Results

Predicted value: 51.0 °C

Global applicability domain: Inside

Local applicability domain index: 4.80e-01

Confidence level: 4.77e-01

Nearest Neighbors from the Training Set

Image not found
Allethrin
Measured: -40.0
Predicted: -20.4

Image not found
Sebacil
Measured: 40.5
Predicted: 16.6